

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053024\
 Data File : VU059092.D
 Acq On : 30 May 2024 14:27
 Operator : MD/SY
 Sample : P2623-01ME
 Misc : 5.12g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHBQ8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

Signal : TIC: VU059092.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	86	94	119	rVB	69932	98302	13.27%	1.640%
2	1.830	136	168	169	rBV3	57185	207483	28.02%	3.462%
3	2.544	379	390	409	rVB	137028	222345	30.02%	3.710%
4	2.624	411	415	420	rBV5	712	890	0.12%	0.015%
5	2.772	452	461	467	rBV4	852	1353	0.18%	0.023%
6	3.030	533	541	551	rBV3	2744	4623	0.62%	0.077%
7	3.100	560	563	567	rVB2	337	244	0.03%	0.004%
8	3.168	573	584	600	rBV2	3934	9941	1.34%	0.166%
9	3.274	614	617	620	rBV3	250	204	0.03%	0.003%
10	3.669	732	740	741	rBV2	397	345	0.05%	0.006%
11	4.206	903	907	914	rVB2	369	454	0.06%	0.008%
12	4.239	914	917	922	rBV	238	231	0.03%	0.004%
13	4.341	946	949	954	rVB2	246	261	0.04%	0.004%
14	4.512	999	1002	1004	rBV	291	221	0.03%	0.004%
15	4.570	1016	1020	1024	rVB2	256	230	0.03%	0.004%
16	4.618	1024	1035	1072	rBV	57940	173206	23.39%	2.890%
17	5.049	1153	1169	1188	rBV2	129264	288313	38.93%	4.810%
18	5.226	1218	1224	1225	rBV2	214	205	0.03%	0.003%
19	5.277	1235	1240	1243	rBV3	251	211	0.03%	0.004%
20	5.711	1355	1375	1405	rBV2	276755	740578	100.00%	12.356%
21	5.830	1409	1412	1415	rVB	512	348	0.05%	0.006%
22	5.849	1415	1418	1420	rBV2	274	195	0.03%	0.003%
23	5.923	1437	1441	1444	rBV2	314	306	0.04%	0.005%
24	5.972	1448	1456	1461	rBV4	1819	2992	0.40%	0.050%
25	6.026	1469	1473	1476	rBV2	396	335	0.05%	0.006%
26	6.042	1476	1478	1485	rVB3	304	253	0.03%	0.004%
27	6.084	1486	1491	1495	rVB2	282	333	0.04%	0.006%
28	6.110	1495	1499	1503	rBV2	205	202	0.03%	0.003%
29	6.139	1503	1508	1512	rBV2	322	323	0.04%	0.005%
30	6.238	1524	1539	1565	rBV	259680	504683	68.15%	8.420%
31	6.451	1603	1605	1610	rVB2	226	199	0.03%	0.003%
32	6.528	1617	1629	1640	rBV7	5184	9839	1.33%	0.164%
33	6.595	1640	1650	1654	rBV5	2340	3918	0.53%	0.065%
34	6.682	1664	1677	1706	rBV2	168895	336912	45.49%	5.621%
35	6.820	1716	1720	1722	rVB2	310	199	0.03%	0.003%
36	6.885	1736	1740	1743	rVB2	240	225	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053024\
 Data File : VU059092.D
 Acq On : 30 May 2024 14:27
 Operator : MD/SY
 Sample : P2623-01ME
 Misc : 5.12g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHBQ8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

37	6.907	1743	1747	1750	rBV2	200	217	0.03%	0.004%
38	7.029	1783	1785	1789	rVB2	284	211	0.03%	0.004%
39	7.103	1804	1808	1812	rBV2	217	213	0.03%	0.004%
40	7.200	1830	1838	1839	rBV2	731	727	0.10%	0.012%
41	7.274	1857	1861	1864	rBV	292	299	0.04%	0.005%
42	7.361	1885	1888	1895	rVB2	280	237	0.03%	0.004%
43	7.560	1938	1950	1969	rBV2	84695	157708	21.30%	2.631%
44	7.714	1994	1998	2000	rBV2	299	193	0.03%	0.003%
45	7.788	2015	2021	2024	rBV	382	488	0.07%	0.008%
46	7.891	2040	2053	2074	rBV	312916	551184	74.43%	9.196%
47	8.123	2122	2125	2129	rVB2	259	204	0.03%	0.003%
48	8.174	2129	2141	2160	rBV	58883	108676	14.67%	1.813%
49	8.299	2175	2180	2183	rVB2	371	304	0.04%	0.005%
50	8.338	2188	2192	2193	rBV2	398	233	0.03%	0.004%
51	8.373	2200	2203	2206	rBV2	254	212	0.03%	0.004%
52	8.393	2206	2209	2214	rVV2	217	219	0.03%	0.004%
53	8.460	2222	2230	2231	rBV2	620	634	0.09%	0.011%
54	8.566	2258	2263	2265	rBV2	257	251	0.03%	0.004%
55	8.582	2265	2268	2272	rVB2	327	295	0.04%	0.005%
56	8.637	2272	2285	2323	rBV2	154635	367503	49.62%	6.132%
57	8.820	2337	2342	2343	rBV2	390	267	0.04%	0.004%
58	8.904	2365	2368	2376	rVB3	316	363	0.05%	0.006%
59	8.981	2389	2392	2397	rVB2	238	232	0.03%	0.004%
60	9.045	2408	2412	2418	rVB2	277	284	0.04%	0.005%
61	9.412	2514	2526	2552	rBV	379417	663500	89.59%	11.070%
62	9.560	2567	2572	2574	rBV2	372	289	0.04%	0.005%
63	9.579	2574	2578	2585	rVB2	665	626	0.08%	0.010%
64	9.692	2608	2613	2614	rBV2	920	754	0.10%	0.013%
65	9.766	2634	2636	2639	rVV2	329	215	0.03%	0.004%
66	9.984	2701	2704	2708	rBV2	249	292	0.04%	0.005%
67	10.103	2739	2741	2747	rVB3	424	345	0.05%	0.006%
68	10.177	2760	2764	2770	rVB2	202	227	0.03%	0.004%
69	10.299	2795	2802	2806	rBV2	296	359	0.05%	0.006%
70	10.431	2840	2843	2846	rBV2	226	208	0.03%	0.003%
71	10.640	2905	2908	2912	rVB2	271	248	0.03%	0.004%
72	10.663	2912	2915	2919	rBV	333	280	0.04%	0.005%
73	10.753	2930	2943	2971	rVB	241782	404946	54.68%	6.756%
74	11.000	3015	3020	3023	rVB2	281	258	0.03%	0.004%
75	11.055	3033	3037	3039	rBV	264	231	0.03%	0.004%
76	11.097	3047	3050	3055	rBV2	235	197	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053024\
 Data File : VU059092.D
 Acq On : 30 May 2024 14:27
 Operator : MD/SY
 Sample : P2623-01ME
 Misc : 5.12g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHBQ8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

77	11.296	3109	3112	3115	rBV	300	230	0.03%	0.004%
78	11.315	3115	3118	3129	rVB2	319	498	0.07%	0.008%
79	11.357	3129	3131	3135	rBV	200	195	0.03%	0.003%
80	11.518	3177	3181	3185	rVB	376	342	0.05%	0.006%
81	11.807	3259	3271	3297	rBV	372106	611772	82.61%	10.207%
82	11.965	3318	3320	3323	rVB2	422	229	0.03%	0.004%
83	12.061	3347	3350	3354	rVB	292	207	0.03%	0.003%
84	12.190	3378	3390	3412	rBV	296891	499575	67.46%	8.335%
85	12.370	3442	3446	3453	rVV4	452	592	0.08%	0.010%
86	12.479	3478	3480	3484	rBV2	220	193	0.03%	0.003%
87	12.611	3517	3521	3523	rBV	270	219	0.03%	0.004%
88	12.627	3523	3526	3529	rVV	328	216	0.03%	0.004%
89	12.766	3562	3569	3572	rBV2	541	487	0.07%	0.008%
90	12.907	3610	3613	3615	rBV	363	253	0.03%	0.004%
91	12.971	3631	3633	3638	rVB	283	225	0.03%	0.004%
92	13.167	3692	3694	3701	rVB2	367	334	0.05%	0.006%
93	13.865	3908	3911	3914	rBV2	294	234	0.03%	0.004%
94	14.087	3977	3980	3983	rVB3	455	338	0.05%	0.006%
95	14.135	3989	3995	3999	rBV2	316	410	0.06%	0.007%
96	14.161	3999	4003	4007	rVB3	603	496	0.07%	0.008%
97	14.431	4082	4087	4092	rBV2	474	565	0.08%	0.009%
98	14.573	4128	4131	4134	rBV2	501	340	0.05%	0.006%
99	15.116	4296	4300	4302	rBV3	345	267	0.04%	0.004%
100	15.807	4513	4515	4518	rBV	499	263	0.04%	0.004%

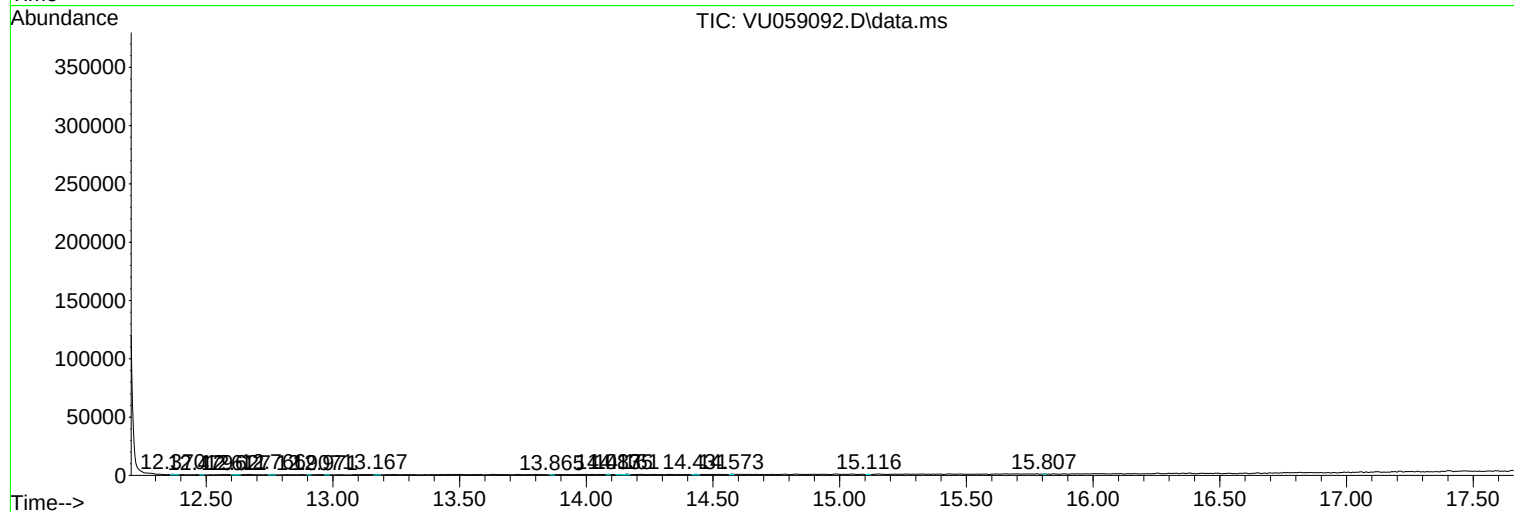
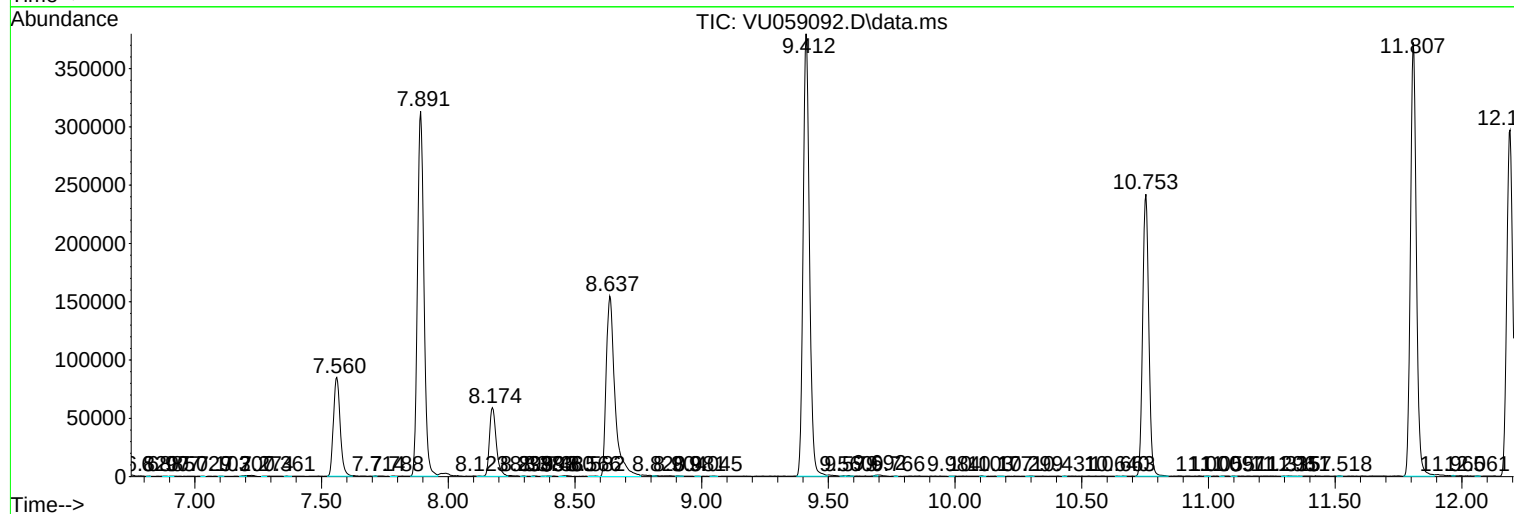
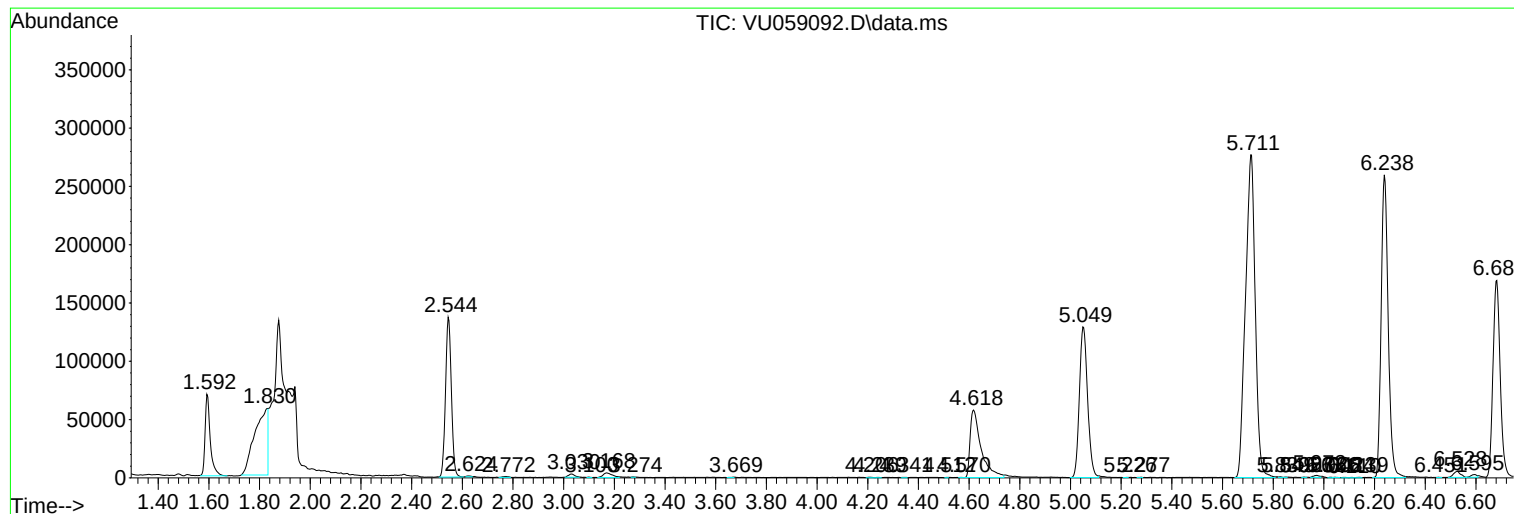
Sum of corrected areas: 5993511

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053024\
Data File : VU059092.D
Acq On : 30 May 2024 14:27
Operator : MD/SY
Sample : P2623-01ME
Misc : 5.12g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHBQ8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053024\
Data File : VU059092.D
Acq On : 30 May 2024 14:27
Operator : MD/SY
Sample : P2623-01ME
Misc : 5.12g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHBQ8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053024\
Data File : VU059092.D
Acq On : 30 May 2024 14:27
Operator : MD/SY
Sample : P2623-01ME
Misc : 5.12g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHBQ8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
------------------	----	---------	-------	----------	---	----	------	------